REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*

2. REPORT TYPE
Technical Papers

3. DATES COVERED *(From - To)*

4. TITLE AND SUBTITLE

Please see attached

5a. CONTRACT NUMBER
In-House

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER
61102F

6. AUTHOR(S)

5d. PROJECT NUMBER
2308

5e. TASK NUMBER
M19B

5f. WORK UNIT NUMBER
346058

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

Air Force Research Laboratory (AFMC)
AFRL/PRS
5 Pollux Drive
Edwards AFB CA 93524-7048

8. PERFORMING ORGANIZATION REPORT

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)

Air Force Research Laboratory (AFMC)
AFRL/PRS
5 Pollux Drive
Edwards AFB CA 93524-7048

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S NUMBER(S) AFRL-PR-ED-TP-2000-162

12. DISTRIBUTION / AVAILABILITY STATEMENT

Approved for public release; distribution unlimited.

13. SUPPLEMENTARY NOTES

14. ABSTRACT

20030310 129

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Leilani Richardson
Unclassified	Unclassified	Unclassified	A		19b. TELEPHONE NUMBER (include area code) (661) 275-5015

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std. 239.18

2308m19B

√DB

MEMORANDUM FOR PRS (In-House/Contractor Publication)

FROM: PROI (TI) (STINFO) 07 Aug 2000

SUBJECT: Authorization for Release of Technical Information, Control Number: **AFRL-PR-ED-TP-2000-162**
I. J. Wysong (AFRL/PRSA); D. C. Wadsworth, D. B. VanGilder (ERC); C. Kaplan, D. Mott (NRL/LCPFD), "SUPREM-DSMC (CHSSI CFD-8) Software Acceptance Test Review (Draft)"

HPCMO CHSSI Software Acceptance Test Review **(Statement A)**
(Washington DC, 11 Aug 00) (Submission Deadline: 10 Aug 00)

SUPREM-DSMC
(CHSSI CFD-8)
Software Acceptance Test Review

Agenda:
- Introduction and Overview: I. Wysong
- Software Design: D. Wadsworth
- Grid and Geometry: C. Kaplan
- Particle Movement: C. Kaplan
- Gas/Chemistry: D. Wadsworth
- Boundary Conditions: D. Wadsworth
- Status and Conclusions: I. Wysong

HPCMO/NRL
Washington, D.C.

11 August, 2000

Computational Fluid Dynamics CTA
(Computational Technology Area)

CTA Leader: Dr. Jay Boris

CFD-8: SUPREM DSMC

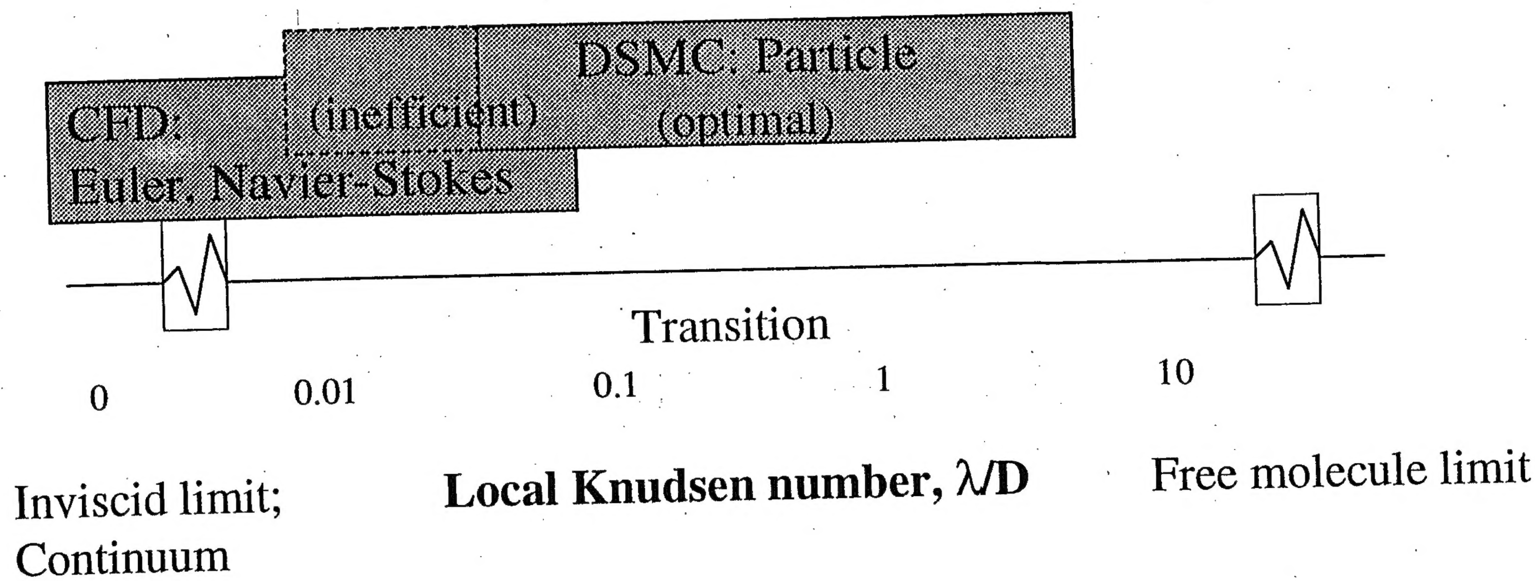
Scalable, Parallel, Reacting, Multidimensional Direct Simulation Monte Carlo Flow Code

Awarded: November, 1999

Start Date: January, 2000

Direct Simulation Monte Carlo method (DSMC)

- Reduced number of model particles represent real gas
- Moved in a grid covering physical space
- Inter-molecular collisions selected statistically from particles in grid cell; physics and chemistry of collisions modeled directly (but phenomenologically)
- No assumption of equilibrium (e.g., N-S eqns.)

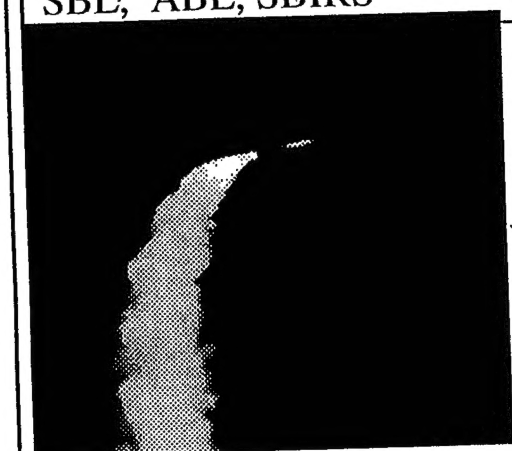


Based on G.A. Bird, "Molecular Gas Dynamics and the Direct Simulation of Gas Flows"

DoD Need for DSMC Simulation Capability:

BattleSpace Environment Simulation codes:

NTW, THAAD, NMD, SBL, ABL, SBIRS



Plasma Processing (etching, deposition, wafer yield):

Intel, Watkins-Johnson

Micropropulsion, MEMS (microfluidics):

AF, NASA (JPL), DARPA

Hypersonic Re-entry Vehicles

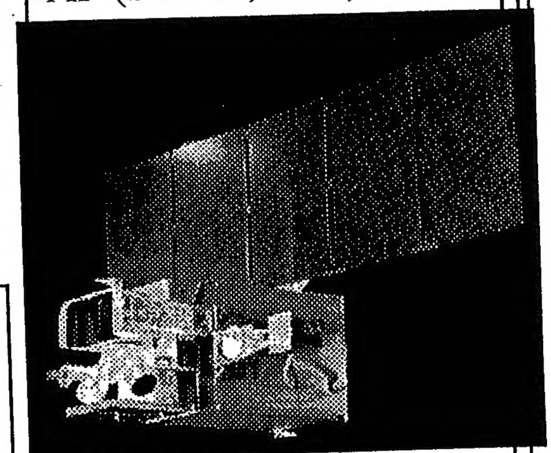
(heat transfer, drag…):

NASA (planetary probes, shuttle), AF(HyTech, Military Aerospace Vehicle)

insert space

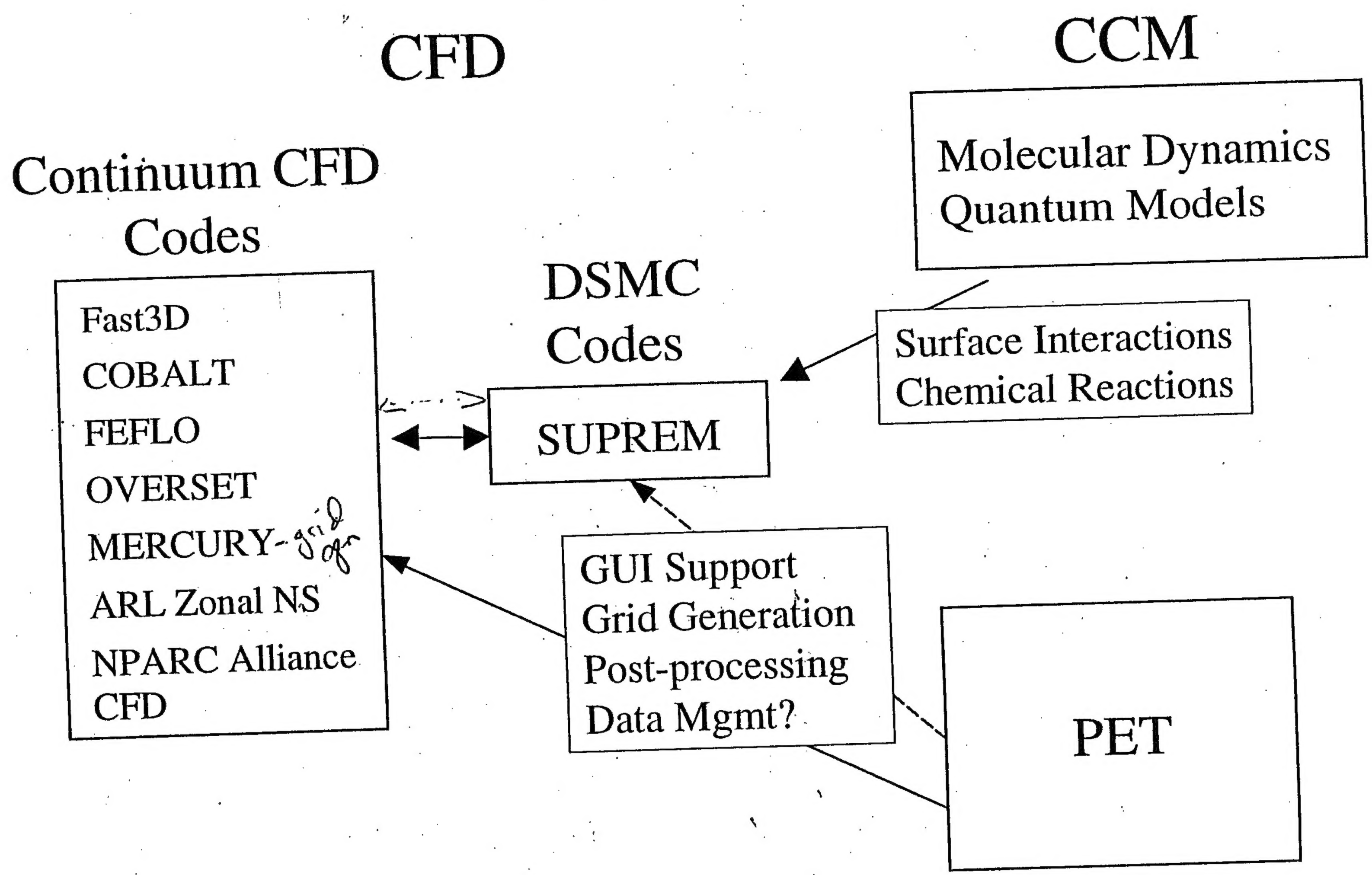
Spacecraft Contamination (lifetime on orbit):

AF (SBIRS, SBL), NASA



X

Integration into HPCMO CHSSI Program



SUPREM Team:

AFRL/PRSA (Edwards AFB, CA):
Dr. Ingrid Wysong
Dr. Dean Wadsworth
Dr. Douglas VanGilder
Dr. David Campbell

Code architecture
User Interface, automation
Particle collisions
Boundary Conditions, Sampling
Chemical reaction & species databases

NRL/LCP (Washington, DC):
Dr. Carolyn Kaplan
Dr. Elaine Oran
Dr. David Mott

Grid
Geometry
Particle movement through grid
Parallelization

Consultants: International Team of DSMC Experts:
Prof. Graeme Bird (Sydney, Australia)
Prof. Mikhail Ivanov (Inst. Theor. Appl. Mech., Novosibirsk, Russia)
Prof. Iain Boyd (Univ. Michigan)

SUPREM Team: Project Management

- Geographically distributed:
  - inter-service team brings greater range of experience and breadth of DoD resources.
  - Real-time interaction limited: face-to-face meetings infrequent. Thus, use of email, video and telephone conferences important.

remove extra space

- Software configuration management:
  - Problems:
    - Not a mature process (No HPC MSRC Provision)
    - Single vs. multiple distributed repositories
    - DSMC is "toolbox", i.e., complex input, many models
  - Solution: Aegis (Gnu)
    - 1 version of code
    - changes undergo development, build, test, review, integration
    - each site has repository, synchronized weekly

DSMC Code Availability

- Number of research & specialized application codes exist.
- None optimized for DoD RDT&E community.

Code: Funding	Ser/ Par.	Geom.	Grid	Lang.	User Interface	Documentation
Socrates: AF/BMDO	S	3D	Cartesian Static	F77	Text/ Windows	User, Theory
Bird: COTS	S	2D/3D	Cartesian Adaptive	F77	Windows	(user), (theory)
SMILE:	P	2D/3D	Cartesian Adaptive	F77/C	Text/GUI	(user), (theory)
Monaco: Univ.	P	2D/3D	Unstruct. Static	F77/C	Text files	(user)
DAC: NASA	P	3D	Cartesian Static	F77	Text	-
SUPREM: HPCMO	P	3D/2D	Cartesian Adaptive	F90	Text/GUI	User, Theory, & Prog.

X

SUPREM: Capability Assessment/Feedback

- Detailed DoD User Requirements:

Questionnaire emailed to users, potential users and DSMC researchers

- Direct Discussions and Input from Users:

AIAA Reno, Jan 00; JANNAF, May 00; AIAA Denver June 00

- Direct Discussions with consultants:

AIAA, Reno, Jan 00; AIAA Denver, June 00

SUPREM Approach

Primary requirements: Robust, reliable performance and results for non-expert users (efficiency secondary)

- HPC
  - Language: Fortran 90 + MPI [possibly HPF-2]
    - dynamic memory & portable
  - Platforms: Initial version to be demonstrated on SGI-Origin, IBM-SP. Then portable to other platforms.
- Software
  - Structured, Modular, Modern code and coding practices to enable flexibility and upgradability. (supplemented by documentation).
  - Hierarchical design:
    - input/interface
    - data structures

X

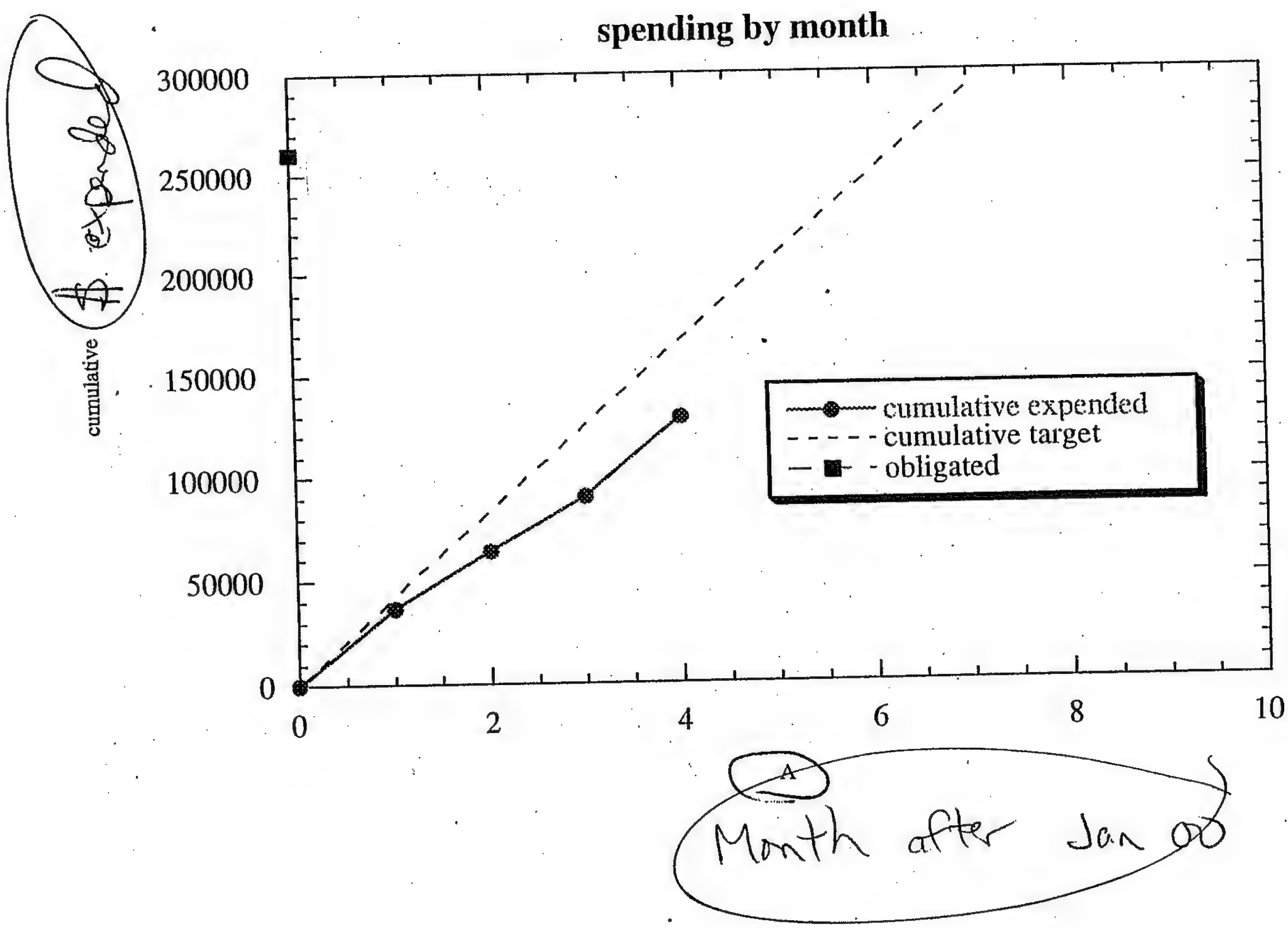
SUPREM: Risk Mitigation

- Build on DSMC core modules and experience of AFRL and NRL teams.
- Input from expert advisory panel.
- Use thoroughly established and tested algorithms.
- Validation of results against established data sets, analytical cases and extent research codes.
- Frequent input from DoD users to ensure product will meet requirements. (Tech. transitions/ leveraging).

SUPREM: Leveraging

- BMDO -- plume simulation expertise, potential additional funding for radiation module
- NRL DARPA-funded MEMS-flow computations
- AFRL AFOSR-funded research into DSMC collision models and validation cases
- Spectral Sciences SBIR project: comparison case runs for molecular beam simulation, unsteady flowfield computational techniques

CFD-8 Spending Profile



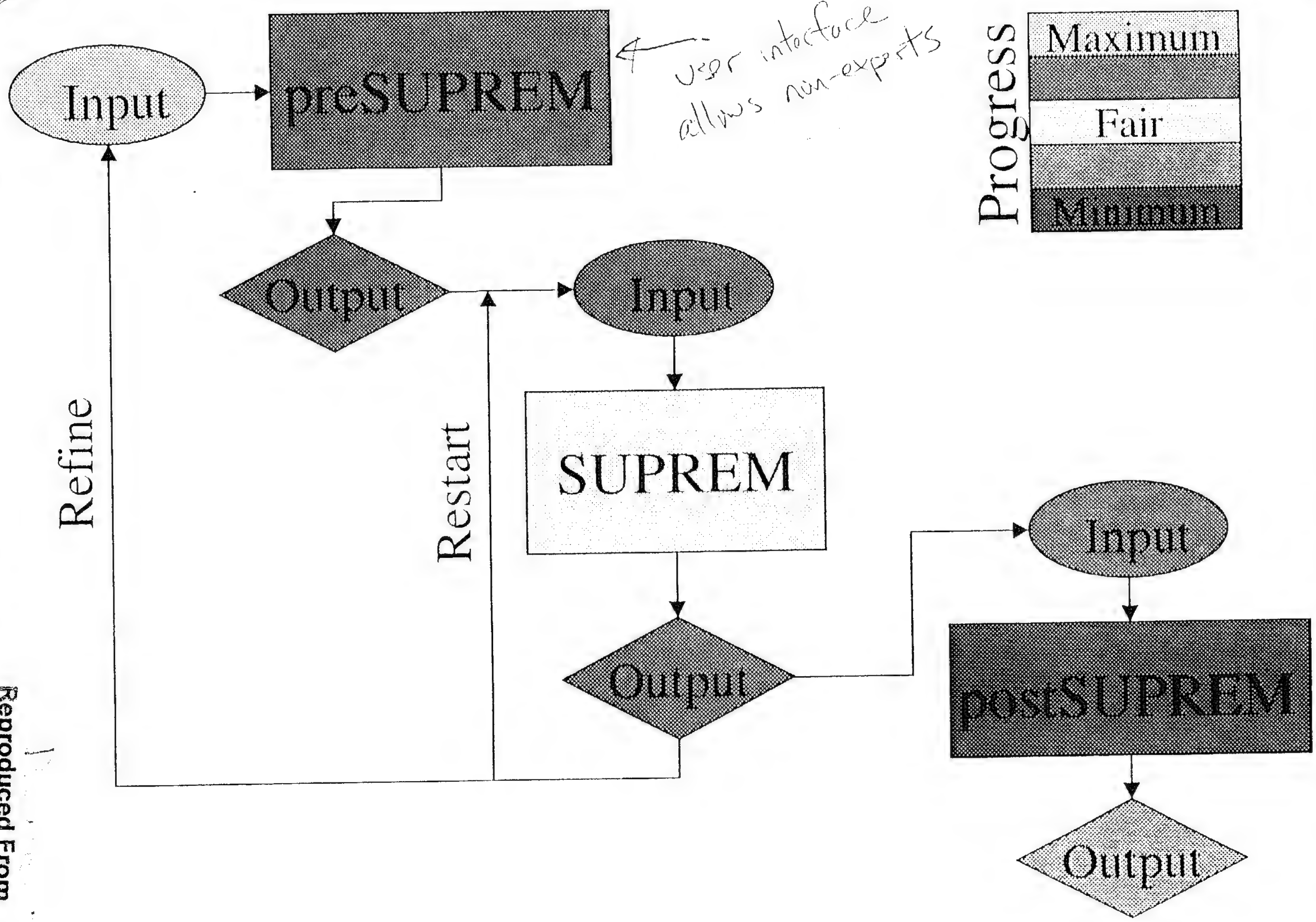
?

update

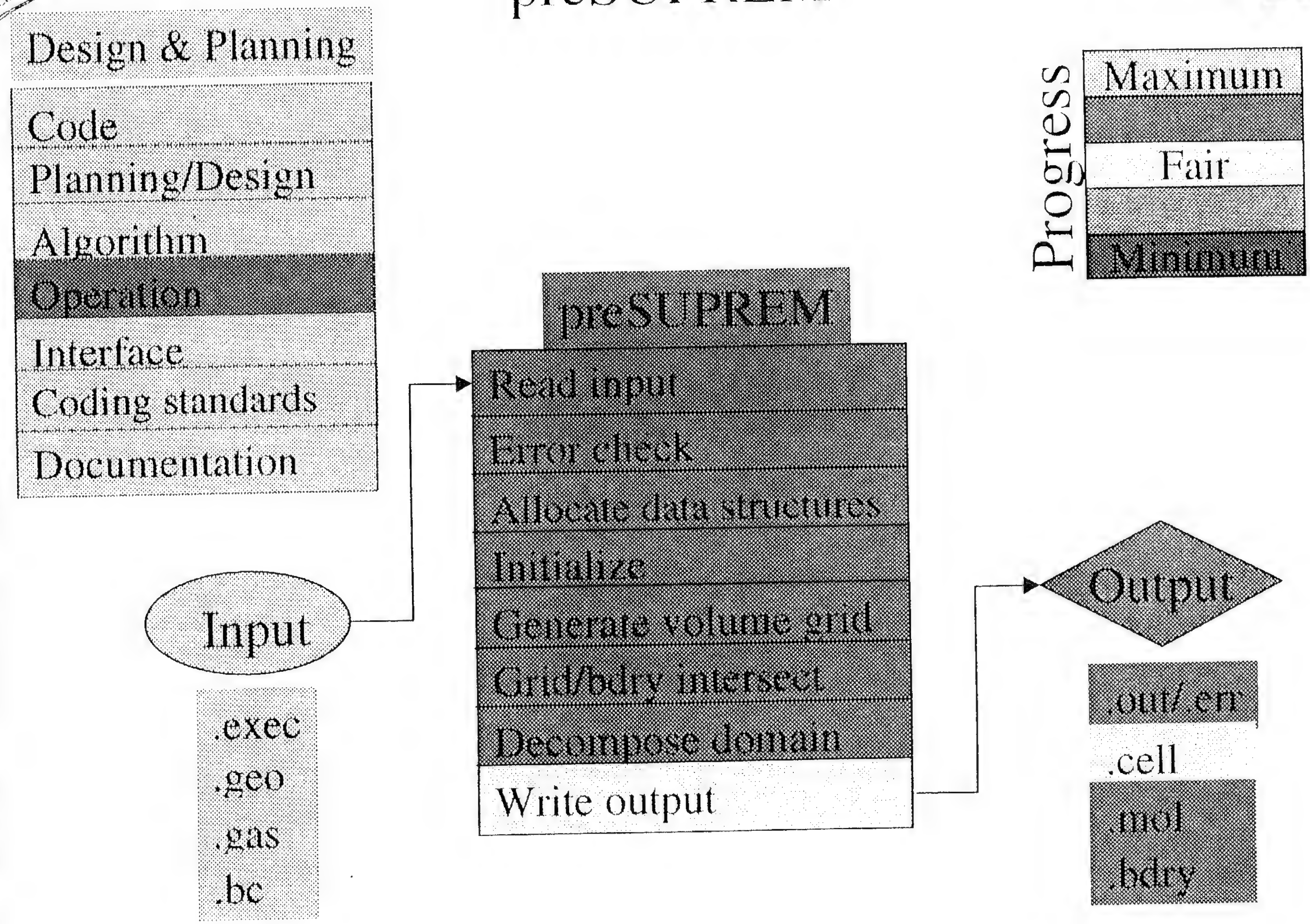
SUPREM DSMC Scalable, Parallel, Reacting, Multidimensional Direct Simulation Monte Carlo Flow Code	FY00				FY01				FY02				FY03		
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3
SAT, TEMP Addendum		◆													
Modules 1-11*, Template			◆												
SAT			◆												
Initial Scalable					◆										
Modules 1-11*, Alpha capability							◆								
Initial Demo Problems, 2-D							◆								
Alpha Test Review							◆								
Alpha Release							◆								
Modules 1-11, Beta capability											◆				
Demo Problems, 3-D											◆				
Initial Documentation											◆				
Beta Test Review											◆				
Beta Release											◆				
Modules 1-11*, IOC capability													◆		
Final Validation and Documentation													◆		
IOTE													◆		
IOC													◆		
Funding Profile Appropriation: PE: Ore: Prog:	$375,000				$500,000				$500,000				$125,000		

scale

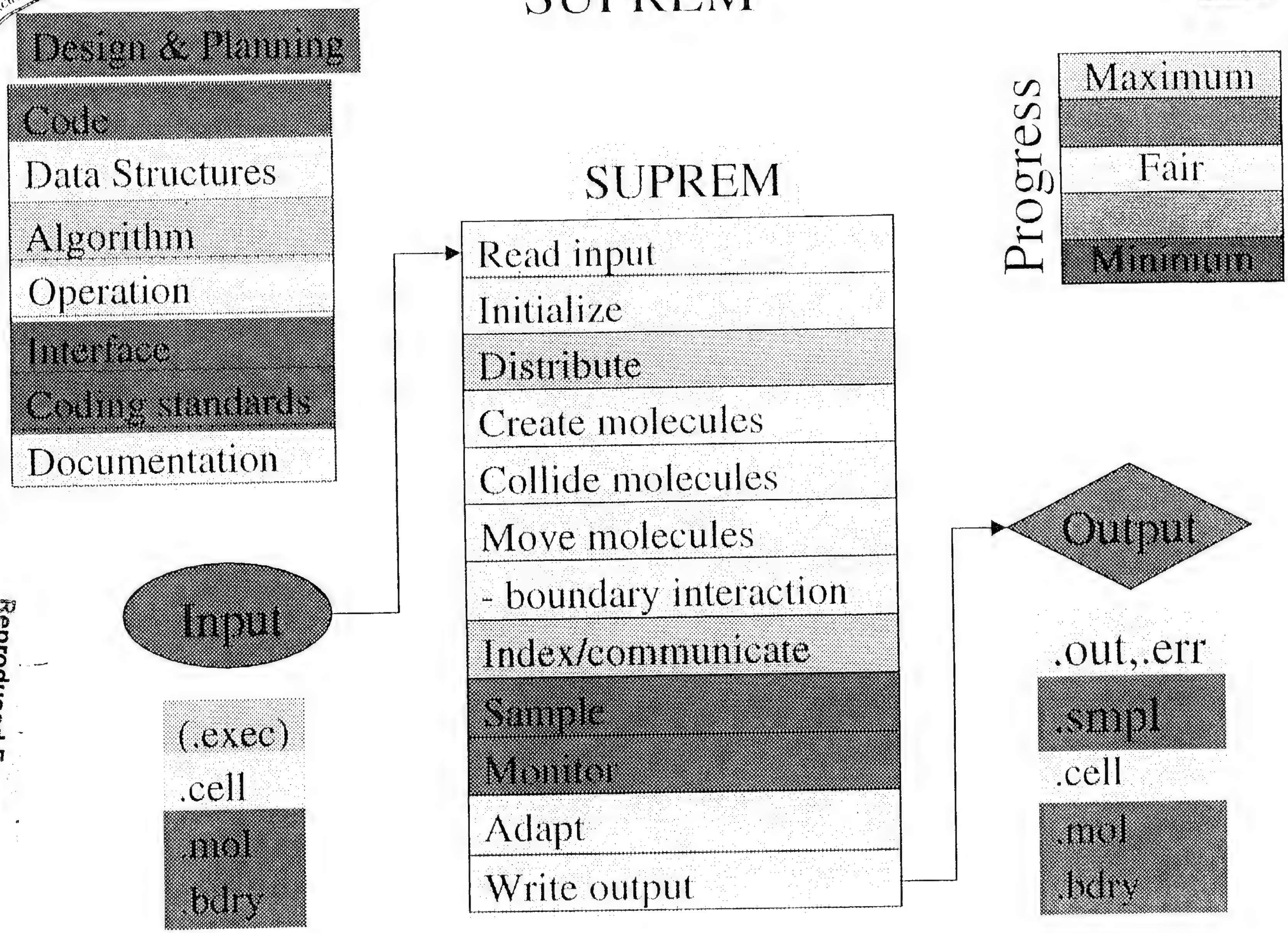
SUPREM-DSMC Overview & Status



Code Overview & Status: preSUPREM



Code Overview & Status: SUPREM



Software Design

- Configuration Management
- User Interface / Code Operation
- Automation / Adaption

Configuration Management

- One Active, Validated Version of Code (Baseline)
- Configuration Management Process:
  - At Minimum: Source Code Version Control
  - Develop / Modify / Build / Test / Review ...
  - Integrate Changes into Baseline
  - Distribute
  - Track Bugs / Fixes
- Desire to Leverage HPC/CHSSI/PET in this Area
  - No CHSSI/PET/MSRC Process Identified
  - MSRC Serves as Repository of Application Codes (Executables)
  - Need "Standards" - Repository of Software Development / Maintenance Expertise

Configuration Management (cont.)

- Aegis (GNU) Selected as C.M. Tool (and C. M. Process)
  - Multiple Architecture Support
  - Full Regression Testing is Integral
- Multiple Local Repositories (ARFL, NRL)
- Changes "Pushed" Weekly
- Repository Includes (& Aegis *Controls*):
  - Source code, etc,
  - Documentation
  - Databases (Gas, Chemistry, etc.)
  - Test, Demonstration, Validation Cases & Results

Coding Standards

- Modularity / Extendibility of Source Code and Data Structures is Key Objective check spacing between lines
  - Object-Oriented
  - Data-Hiding
  - Data-Proximity
- Exploit Fortran90 [HPF-2?] Features
  - Modules
  - Interfaces
  - Data Structures (TYPE)
  - Parallel Portability / Maintainability (HPF-2)
- Establish Templates for Key Modules / Routines
  - Standardization
  - Re-use
- Data Management?
  - Database Format (HDF/CGNS?) / Interface to External Tools

User Interface

- DSMC as Toolbox
  - Grows in Complexity with Time (“Feature Creep”)
  - No Single or Optimal Approach / Algorithm / Model
  - Robustness Makes Maintenance / Control Difficult
- Provide / Enforce Standardized Interface
  - Scalable Physics - Models Classed by Complexity
  - Restrict Features Based on User Expertise
  - Very Complex Input - Automate or Guide Problem Setup
- Control Size / Contents / Usage of Toolbox

User Interface (cont.)

- Hierarchical / Extendable Input
- User Expertise versus Code Features
  - Novice: Restricted Access, Limited Control (Automatic, Conservative Defaults)
  - Intermediate
  - Expert: Full Access, Full Control
- "Problem Type" versus Setup and Model Availability
  - Dominant Flowfield Characteristics (Shock Layer, etc.) can be used to Guide Selection of Models (Gas, Chemistry, Boundary Conditions, Grid, etc.)

Automation

- User Defines Problem, but Code Should Control How Solution is Obtained
- Are the Results Accurate?
  - Satisfy DSMC Algorithm
    - Time Step, Cell Size, Nearest-Neighbor Collision Partners
  - Satisfy Physics of Problem
    - Gas Representation, Chemistry, Boundary Conditions
- Is the Simulation Efficient?
  - Memory, CPU, Load Balance
- Primary Objective: Accuracy, Generality, Scalability, and Robustness of Physics and Algorithm

Automation (cont.)

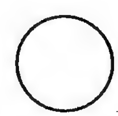
- Very Limited Existing DSMC Work in this Area - Far Short of Conventional CFD
- Plan:
  - – Quality / Accuracy Constraints Represented via Metrics
    - Global (Average)
    - Local (Worst Case)
  - – Expert User (Only) Can Tradeoff Quality for Efficiency
  - – Interpretation of Results Facilitated by Feedback & Output
    - Desired vs. Achieved Quality and Accuracy Metrics
    - Refinement / Adaptation Results

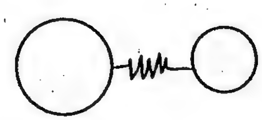
Gas / Chemistry Description

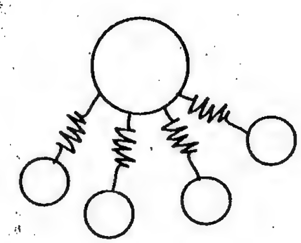
- Representation
- Models
- Algorithms
- Data Structures
- User Access
  - Input
  - Initialization
  - Sampling/Output

Gas Model

- Multiple Species
- Arbitrary Complexity of Each (Scalable)
  - Number of Independent Internal Modes
  - Representation of Mode (Continuous or Quantized)
  - Each Mode is a Scalar Quantity Stored for Each Molecule

Atom  Ar (ε_t)

Diatom  NO ($\varepsilon_t, \varepsilon_r, \varepsilon_v$)

Polyatom  CH_4 ($\varepsilon_t, \varepsilon_{r1} .. \varepsilon_{rn}, \varepsilon_{v1} .. \varepsilon_{vn}$)

Gas Model

- Predefined Common Modes are Available
  - Rotation -- Rigid Rotor: Quantized, Bounded

    $\varepsilon_j = k_B \theta_r j(j+1)$ gives ε_r for level j
  - Vibration -- Simple Harmonic Oscillator: Quantized, Bounded
    - Anharmonic Oscillator: Quantized, Bounded
- Allow Fictitious or Simplified Representation
  - Lumped -- Combine (Lump) "Real" Modes Together
  - Arbitrary Subset of Levels in a Quantized Mode

Databases Provided for Common Applications

X

- Completeness/Complexity Parameterized by Flow Energy Content (e.g., Temperature, Velocity, Average Collision Energy) Relative to Characteristic Mode Energy
- Simple Monatomics
  - e.g., Ar
- Common laboratory species
  - N_2
    - Room Temperature / Thermal
    - Weak or Strong Shock Layers
- Air
  - N_2, O_2
  - N_2, O_2, O, N, NO
- Propellents, Combustion Products
  - CO, CO_2, CH, H_2O

Access to Molecules / Species

- Input: Compact, Self-contained Definition Section; 1 for Each Species
- Initialization: Molecule of a Given Species can be Assigned an Arbitrary Velocity & Energy in any mode
  - Sampled from Equilibrium (e.g., Temperature)
  - Sampled from Nonequilibrium Distribution (e.g., Discrete Mode Energy Population)
- Sampling/ Output:
  - Default: Mean Properties per Mode in ALL Cells
  - "Detail": Distribution Function of Any Mode of Any Species (at Any Location) -- Vital for "Microscopic" Interpretation

Molecule and Species Data Structures

Molecule

- Species_ID ispec
- XYZ(:)
- VEL(3)
- Mode_energy(:)
- etc.

Species (1..Num_species)

- Name
- Composition
- Mass
- Num_modes
- Modes(1..Num_modes)

Mode

- Name
- Max_energy
- Rep(resentation)
  - Cont(inous)

  or
  - Quant(ized)

Cont

- DOF

Quant

- Num_levels
- Energy(1..nlvls)

Chemistry (Intermolecular Collision) Model

- Bimolecular [Trimolecular & Unimolecular also Available]
- Arbitrary Complexity of Collision for Each Species Pair (Scalable)
  - Number of Independent Processes
  - Complexity of Each Process
- Collision Description is INPUT (Self-Documenting)
  - 1) Chemical Equation:
    - Defines Species and Modes that Participate
  - 2) Process Keyword Description:
    - Type (Elastic, Inelastic, Reaction)
    - Model Used to Calculate Cross Section σ and Model Parameters

Chemical/ Collision Equations

- $NO + O \rightarrow NO + O$
  - PROCESS: ELASTIC
    - VHS, VSS Model Used to Calculate $\sigma_{\mathrm{e}} = \sigma_{\mathrm{e}}(\varepsilon_{\mathrm{t}})$
    - Isotropic Scattering
- $NO(\varepsilon_r) + O \rightarrow NO(\varepsilon_r') + O$
  - PROCESS: INELASTIC
    - Collision Number "Z" Model $\sigma_{\mathrm{i}} = \sigma_{\mathrm{i}}(\varepsilon_{\mathrm{t}}) \approx \frac{1}{z}\sigma_{\mathrm{e}}(\varepsilon_{\mathrm{t}})$
    - Borgnakke-Larsen Redistribution (ε_r')
- $NO(\varepsilon_r, \varepsilon_v) + O \rightarrow N + O_2(\varepsilon_r', \varepsilon_v')$
  - PROCESS: REACTION
    - Total Collision Energy (Arrhenius-based) Model

$$\sigma_r = \sigma_r(\varepsilon_c = \varepsilon_t + \varepsilon_r + \varepsilon_v)$$

    - Borgnakke-Larsen Redistribution/Initialization (ε_r',ε_v')

Collision Representation - Issues

- DSMC Collision Models are Wholly Phenomenological
  - Microscopic/ Kinetic Description Required, but is Nominally Based on Macroscopic Data
  - No Real Cross Sections are Used
- Complex, Real Coupled Processes are Necessarily Decoupled
- Statistical Process: Detailed Balance Achieved by Uncorrelating Pre- & Post- States
- Continued Research into Collision Physics & DSMC-Representation Required
  - SUPREM team
  - CCM

Collision Algorithm - Implementation

- Pair Selection is Cell-Local
  - Nearest-Neighbor Approximated via Bird Transient Adaptive Subcell Procedure
- Pair & Pair-Process Acceptance
  - Independent of Process Type or Input Order
  - Depends ONLY on (Abstract) Physical Parameter σ
- Null Collision Method
  - Probability of Process $P_i = \dfrac{\sigma_i}{\sum_{j=1}^{N} \sigma_j}$

Collision Description - User Issues

- Databases Provided for Common Gases
- User (NOT Black-Box Code) Determines Complexity of Gas & Collision Processes
- Extensive Diagnostics & Feedback from Code
  - DSMC Constraints (e.g., Nearest-Neighbor)
  - Model Realism / Accuracy / Range [Limits] of Applicability

User Access to Collision Processes

- Input: Compact, Self-Documenting for Each Pair / Process
- Initialization: N/A
- Sampling / Output
  - Default: Mean Properties (e.g., Collision Frequencies) Per Pair (& Per Process)
  - Detail: Distribution Function of Any Mode of Any Species (Pre- and/or Post- Collision) -- Vital for Improvement of DSMC Models & Interpretation of Results

Collision Pair Data Structures

Colln_Pair(ispec,jspec)

space ?

- Weight
- Num_processes
- Process(1..Num_processes)

Process

- Type/name
- Modes_involved
- Model

Parameters(1..N)

Gas/ Chemistry Example Input File (Ar-N_2)

1) Species Definition

```
SPECIES_NAME Ar
  COMPOSITION Ar-1
  NUM_INTL_MODES 0
SPECIES_NAME NO
  COMPOSITION N-1 O-1
  NUM_INTL_MODES 2
  MODE_NAME ROT
   MODE_REP  CONTIN
   DOF 2
   MAX_ENERGY 1.04E-17
  MODE_NAME AHOVIB
   MAX_ENERGY 1.04E-17
   NUM_DUNHAM_TERMS 3
   DUNHAM_COEFFS 0.1 0.2 0.3
```

Gas/ Chemistry Example Input (cont.)

2) Collision Definition

```
BIMOLECULAR TRUE
SPECIES_PAIR Ar ANY
 Ar + ANY -> Ar + ANY
    PROCESS ELASTIC  MODEL VHS  NUM_PARAMS 3
      DIAM_REF   4.185e-10
      VISC_EXPON 0.80
      TEMP_REF   273.
      COMMENT ref: Bird 1994, App. A, avg(NO+Ar)"
SPECIES_PAIR NO NO
 NO + NO -> NO + NO
   PROCESS ELASTIC  MODEL VHS  NUM_PARAMS 3
      ...
 NO(ROT) + NO -> NO(ROT') + NO
   PROCESS INELASTIC  MODEL COLLN_NUM  NUM_PARAMS 2
      COLLN_NUM 5.0
      TEMP_REF  300.
SPECIES_PAIR NO Ar
   ...
```

Boundary Conditions

- Describe:
  1. Interaction of Molecule with Boundary During Molecular Movement Stage
  2. Spontaneous Creation of Molecules at Boundary (e.g., Inflow)
- Allow Arbitrary Complexity (Scalable)
  - Define Several Basic Types or Classes (General Characteristics)
  - Each Type has Several Subtypes
    - Simple to Complex
    - Highly Constrained to General / Arbitrary
  - Constant or Prescribed Variation in Space or Time

Boundary Conditions

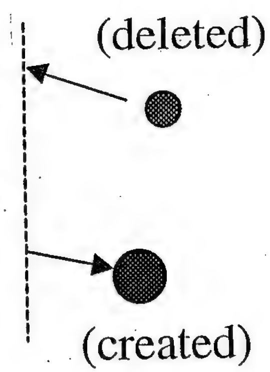
of existing molec.?

Type	Subtype	Interaction	Creation
SOURCE	MACRO	Delete	Constant, Equilibrium
	MSIS90	Delete	Constant, Equilibrium
	MANUAL	Delete	Arbitrary (f(x,y,z), Noneq.)
	MOL_LIST	Delete	[Externally Supplied]
	ITERATIVE	Delete	Adjustable Rate, Equilibrium
SINK	VACUUM	Delete	N/A
	PUMP	Possible Reflection	N/A
WALL		Reflection/Reaction	N/A
	OUTGAS	Reflection/Reaction	Constant, Equilibrium
	DESORB	Reflection/Reaction	Coverage-Dependent, Equilibrium
SYMMETRY		Specular Reflection	N/A
FLUXPLANE		No Change	N/A
PERIODIC	LINEAR	Linear Displacement	[Displ. from matching bdry]
	AZIMUTHAL	Rotational Displ.	[Displ. from matching bdry]

Source Boundary Condition

- Typical Case: Constant Inflow, Known Freestream Macroscopic Properties $(n_\infty, p_\infty, T_\infty, u_\infty)$
- General Case: Arbitrary Spatial Variation (e.g., U Profile), Inter-species, Inter-mode, Intra-mode Nonequilibrium

$\rho_\infty, T_\infty, u_\infty \rightarrow$



Sample u, E_{mode}
- u_∞, T_∞ (Equilibrium)
- $f(u), f(\varepsilon_r), f(\varepsilon_v)$ (Nonequilibrium)

- Issues:
  - Subsonic vs. Supersonic (Directed Fluxes)
  - Macroscopic vs. Microscopic Description

Source / MACRO

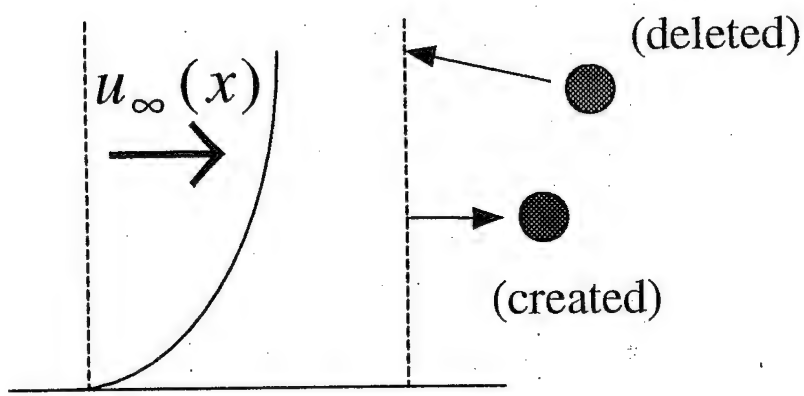
- Constant Incoming (Created) Flux
- Incoming Flux Independent of Outgoing Flux
- Strictly Valid Only for High Supersonic Speeds
- Molecule Properties Sampled from Analytical Equilibrium Kinetic Flux

$$\text{Flux} = n\overline{Qu_n} = n\int_{dv} Qu_n f d\overset{\varpi}{v}; \quad f \propto \exp\left(\frac{-mc'^2}{2k_B T}\right)$$

Flux:	Q =
Mass	m
Momentum	$m\overset{\varpi}{v}$
Energy (Trans.)	$m\,\lvert v\rvert^2$

Source / MANUAL

- Generalized Spatial Variation of $\rho_\infty, T_\infty, u_\infty$
- Independent Properties for Each Species
- Independent Properties for Each Mode
  - $T_{\infty \mathrm{mode}}$ or Distribution/Population
  - (Also $T_{\infty x,y,z}$ or $f(u,v,w)$)
- Incoming Flux Uncoupled from Outgoing



Source / MSIS90

- Flight in Earth Atmosphere
- MSIS90 Model Calculates Freestream Properties from Given Flight Parameters
- Remainder Equivalent to Source / Macro

Source / Iterative

- Couple Incoming & Outgoing Fluxes
- Update Incoming Flux Parameters to Recover Desired Net Flux
- Approximate Subsonic Boundary
- Still Based on Equilibrium, Macroscopic Parameters

X

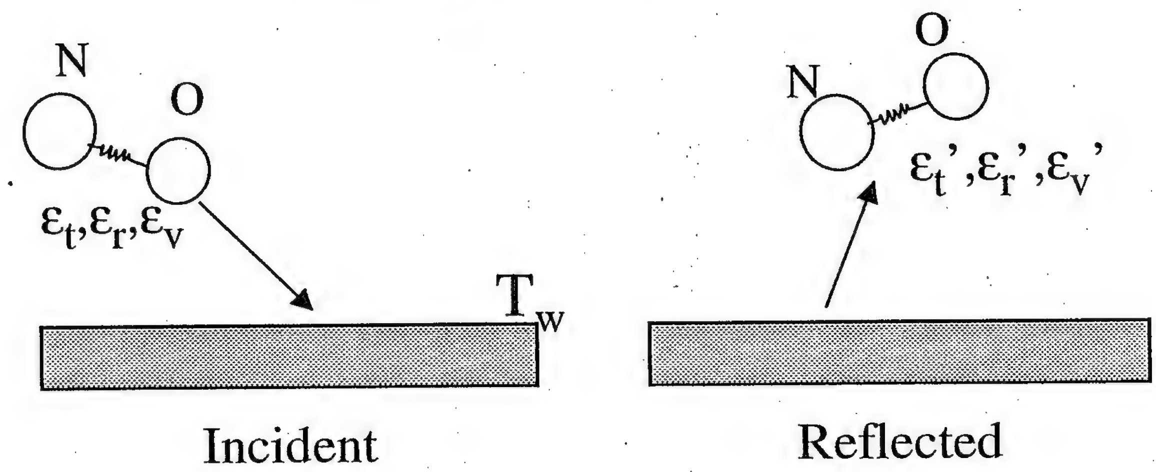
Wall Boundary Condition

- Typical Case: Constant Temperature Engineering Surface (Diffuse, Fully Accommodating Reflection)
- General Case:
  - $T_w(x,y,z)$
  - Species & Mode-Dependent Reflection & Reaction
  - Spontaneous Creation (Outgassing, Desorption)
- Two Components to Description:
  - Properties Associated with Wall Surface
    - Material
    - Temperature, Velocity, Coverage, Spatial Variation
  - Properties Associated with Interaction
    - Process, Model, Parameters

Wall Interaction Processes

- Analogous to Chemistry/Collision Process -
  - Probability (cross-section) of Post-interaction State
- Arbitrary Number and Type of Processes for Each Incident Species / Material Pair (Scalable)
- Interaction Description is Input
  - Chemical Equation - Species & Mode
  - Process Definition
    - Type / Model / Model Parameters

Wall Interaction Equations
Example - Reflection



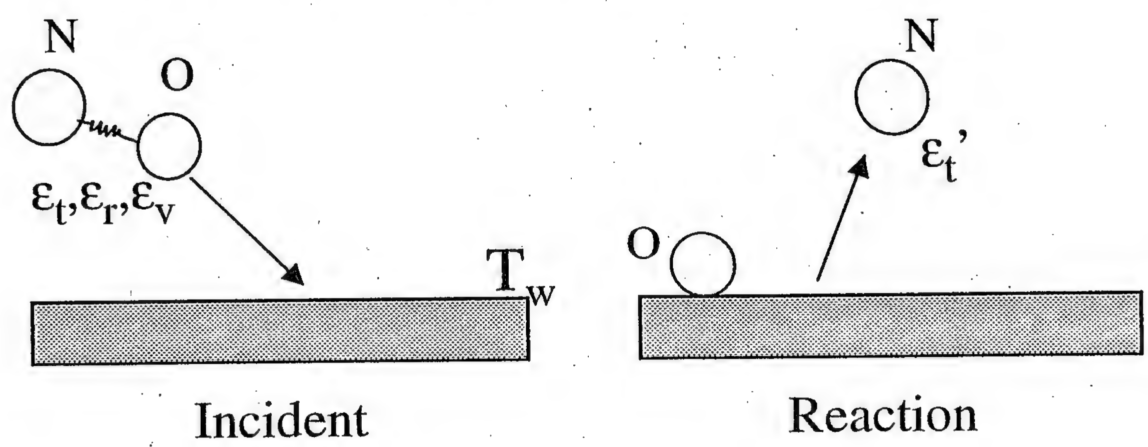
$$NO(\varepsilon_t, \varepsilon_r, \varepsilon_v) + \mathrm{MATL} \rightarrow NO(\varepsilon_t', \varepsilon_r', \varepsilon_v') + \mathrm{MATL}$$

PROCESS RELECTION MODEL MAXWELL NUM_PARAMS 2

PROB_DIFF 0.5

TEMP_REF 300.0

Wall Interaction Equations
Example - Reaction



$$NO(\varepsilon_t, \varepsilon_r, \varepsilon_v) + \mathrm{MATL} \rightarrow N(\varepsilon_t') + \mathrm{MATL}$$

PROCESS REACTION MODEL CATALYTIC NUM_PARAMS 2

PROB_CATALYTIC 0.9

TEMP_REF 1000.0

Wall Interaction Representation Issues

- DSMC Interaction Models are Wholly Phenomenological
  - Microscopic/Kinetic vs. Macroscopic
  - Typically *Independent* of Collision Energy
  - Decoupled from Wall Response
  - Less Sophisticated than Gas-Gas Collision Models
- Much More Research Required
- Present Approach:
  - Implement Available Models
  - Standardize Input & Algorithm
  - Provide Feedback (Accuracy / Realism)

Wall Interaction Algorithm

- Movement Routine Provides:
  - Incident Molecule
  - Boundary Element Involved
- Combination of Serial & Null Collision Schemes
  - Event Probability Independent of Input Order
  - Reflection: Serial, Independent for Each Mode
  - Reaction: Null Collision Evaluation of:

$$\text{Event } i = \frac{p_i}{\sum_{j=1}^{N} p_j}$$

Wall Interaction Description - User Issues

- Very Limited Data for any but "Fully Accommodating, Diffuse Reflection" Process
- User Defines / Controls Complexity of Interaction
- Extensive Feedback
  - DSMC Constraints (Surface Element Size, Sample Size)
  - Model Realism / Accuracy

User Access to Interaction

- Input: Compact, Self-Documenting For Each Species & Process
- Initialization: N/A
- Sampling / Output:
  - Default: Mean Incident and Reflected Species Properties (Fluxes)
  - Detail: Distribution Function of Any Mode of Any Species (Pre- & Post-interaction)
  - Macroscopic: Surface Pressure, Shear
  - Integrated: Forces & Moments on a Component
- (Long Term:) Couple to Material / Surface Response Model